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TRANSPORTATION IN GRAPHS AND THE ADMITTANCE SPECTRUM

Christoph MAAS
Unversität Hamburg, Institut für Angewandte Mathematik, Bundesstr. 55, D-2000 Hamburg 13, Fed. Rep. of Germany

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The admittance spectrum of the underlying graph is used in order to describe the behaviour of a liquid flowing through a system of communicating pipes. The performance of this process enables us to define the 'permeability' of a graph, the 'well-connectedness' of pairs of vertices and the 'good position' of vertices in terms of the second eigenvalue of the admittance matrix and its corresponding eigenvectors. Furthermore, bounds are given for the decrease of the second eigenvalue caused by the insertion of an edge into a graph.

1. Introduction

There are several geographical papers discussing the question, whether important places or well connected sets of towns in a traffic network can be identified by an inspection of certain eigenvalues (e.g. the first one, the second one, the one with the second largest absolute value) and corresponding eigenvectors of e.g. the adjacency matrix of the underlying graph. [4] appears to have been the first major publication on this subject. Other ideas and references can be found in [1] and [5]. In the present paper we shall consider a rather special locomotion process, namely damped oscillations of a liquid in communicating pipes which can be described by the admittance spectrum. From the performance of this process it is possible to deduce a ranking among graphs, among paths between pairs of vertices, or among vertices. In this context the second eigenvalue plays an important role and it is investigated to what extent its decrease caused by the insertion of a new edge into the graph can be predicted.

Other interpretations of the admittance spectrum of a graph are the concepts of a 'combinatorial drum' [2.p. 256] and of the 'algebraic connectivity' of a graph [3].

Notation. Throughout this text $G\ (X,E)$ is an undirected, connected (if not stated otherwise explicitly) graph with vertex set X having n elements $x_1,\dots,x_n$ and edge set E. u, v, w are vectors, and λ, μ, ν always denote eigenvalues.

The *admittance matrix* $D=(d_{ij})_{i,j=1,\dots,n}$ of G is identical to the adjacency matrix outside the main diagonal, whereas on the main diagonal the entries d_{ii} give the negative of the valency of x_i. So every row or column sum in D is zero. All eigenvalues of D are real, and by an easy extension of the Perron–Frobenius theorem on nonnegative matrices [6, Theorem 2.1] it can be shown that D is negative semidefinite and the multiplicity of the eigenvalue zero is equal to the number of components of G.

2. Flow through communicating pipes

Let us imagine a set $X=\{x_1,\dots,x_n\}$ of vertical pipes (which will be called vertices in the sequel) all of the same width, material and height some of which are pairwise connected at their bottoms by horizontal pipes (which will be called edges later) also all having the same characteristics. The horizontal pipes are supposed to be filled completely with a liquid and the vertical ones to be shut at their lower end. If we fill the vertices with the same liquid (every vertex may be filled with a different amount) and then open the connections to the edges at time $t=0$, the liquid will flow along the pipes tending towards a distribution in which every x_i is filled with the same amount of the liquid. We are now looking for the vector-valued function $u(t)$ the i-th component of which gives the quantity (i.e. the height) of liquid in x_i at time t. It is not important what we take as zero level for the values of $u(t)$ as long as it is the same for all x_i. We assume that the zero mark is high enough above the edges so that we can consider them to be at height 'minus infinity'. We also assume that the vertices x_i are long enough so that it never occurs that liquid splashes over the upper end. We then find $u(t)$ as the solution of a system of linear second degree differential equations the following way: The acceleration $[\ddot{u}(t)]_i$ is first of all given by the liquid pressures along all edges ending in x_i. This pressure is (proportional to) the difference in height of the liquid at the endpoints of the edge. The liquid in x_i (measured by $[u(t)]_i$) is diminishing $[u(t)]_i$, the liquid at the other end is increasing it. So this influence is just described by the product of the i-th line of the admittance matrix D of the underlying graph and $u(t)$. The acceleration is diminished by friction in the vertices (the friction in the edges is neglected under the assumption that the edges are very wide and thus the flow is very slow) which is proportional to the velocity $\dot{u}(t)$ with a proportionality factor depending mostly on the liquid chosen and besides that on the material the pipes are made of. Summing up these considerations we get:

$$\ddot{u}(t)=Du(t)-2k\dot{u}(t), \quad k\in R^+ \tag{2.1}$$

with starting conditions $u(0)=v$, $\dot{u}(0)=0$, $v\in R^n$.

This differential equation can be solved explicitly. In the following $0=\lambda_1\geq\lambda_2\geq\cdots\geq\lambda_n$ are the eigenvalues of D and $u^{(1)},\dots,u^{(n)}$ is an orthonormal system of corresponding eigenvectors. The solution then reads:

$$u(t)=\sum_{i=1}^{n}(v,u^{(i)})\cdot u^{(i)}\cdot \mathrm{e}^{-kt}\cdot\varphi_i(t) \tag{2.2}$$

with

$$\varphi_i(t)=\begin{cases}\left(\frac{1}{2}+\frac{k}{2\sqrt{k^2+\lambda_i}}\right)\mathrm{e}^{t\sqrt{k^2+\lambda_i}}+\left(\frac{1}{2}-\frac{k}{2\sqrt{k^2+\lambda_i}}\right)\mathrm{e}^{-t\sqrt{k^2+\lambda_i}} & \text{if } k^2+\lambda_i>0,\\ 1+kt & \text{if } k^2+\lambda_i=0,\\ \cos(t\sqrt{-\lambda_i-k^2})+\frac{k}{\sqrt{-\lambda_i-k^2}}\sin(t\sqrt{-\lambda_i-k^2}) & \text{if } k^2+\lambda_i<0.\end{cases}$$

Let us take a closer look at some expressions.

(i) The term for $i=1$: For every $k>0$ we have $\varphi_1(t)=\mathrm{e}^{kt}$ so the whole term for $i=1$ is always the constant $(\upsilon,u^{(1)})\cdot u^{(1)}$.

(ii) The role of λ_2:

(α) The periodic case. If and only if $(0<)\ k<\sqrt{-\lambda_2}$ holds, for arbitrary starting vectors υ the solution $u(t)$ is a sum of n periodic functions. Roughly speaking, λ_2 produces a bound that k must not exceed in order to enable vibrations in all eigenfrequencies.

(β) The aperiodic case. If and only if $k>\sqrt{-\lambda_n}\ (=\sqrt{\varrho(D)})$ holds, for arbitrary starting vectors υ the solution $u(t)$ is a sum of exponential functions with real exponents and constant coefficients. For $\lambda_2<0$ (i.e. for a connected graph) we have $\lim_{t\to\infty}u(t)=(\upsilon,u^{(1)})u^{(1)}=:\bar{u}$. An estimate for the deviation of $u(t)$ from $\bar{u}$ can be obtained the following way:

$$\begin{aligned}\|u(t)-\bar{u}\|_2&\le\sum_{i=2}^{n}\|(u^{(i)},\upsilon)u^{(i)}\|_2\cdot\mathrm{e}^{-kt}\cdot\varphi_i(t)\\&\le\sum_{i=2}^{n}\|(u^{(i)},\upsilon)u^{(i)}\|_2\cdot\mathrm{e}^{-kt+t\sqrt{k^2+\lambda_i}}\\&\le\left[\sum_{i=2}^{n}\|(u^{(i)},\upsilon)u^{(i)}\|_2\right]\cdot\mathrm{e}^{t(-k+\sqrt{k^2+\lambda_2})}.\end{aligned}$$

Let

$$\tau:=\frac{-\ln 2}{-k+\sqrt{k^2+\lambda_2}}\,.$$

For every t the approximation of $u(t)$ to $\bar{u}$, we can guarantee, is reduced by one half during the time interval from t to $t+\tau$. Therefore we define τ to be the half-life of the flowing-process in the graph. The only one of its parameters stemming from the structure of the graph is λ_2. (The definition of τ makes sense even when $\lambda_2=0$, i.e., the graph has at least two components: As no liquid can flow from one component to another, it can take 'infinitely long' time to make any progress towards $\bar{u}$.)

Up to now we have described the flow of a liquid through a system of communicating pipes. We shall now use these results to classify graphs and certain substructures of theirs according to how well the convergence of $u(t)$ towards the limit vector, i.e., towards the same height of the liquid in all vertices x_i, takes place. To this purpose we shall assume that the viscosity of the liquid is high enough to ensure the presence of the aperiodic case.

3. Classification of graphs

For every connected graph G with n vertices in any orthonormal system of eigenvectors the vector corresponding to $\lambda_1=0$ is $u^{(1)}=(1/\sqrt{n})(1,\dots,1)^{\mathrm{T}}$. All starting-vectors v having the same scalar product $(u^{(1)},v)$ start a process $u(t)$ leading to the same limit $\bar{u}$. So the performance of this process can be measured by the speed of its convergence.

(a) *Permeability of graphs.* If two graphs have the same number of vertices, identical starting-vectors lead to identical limits. We call a graph the more permeable the shorter the half-life of the egalization process is. So we can measure the permeability of a graph by the absolute value of its second largest eigenvalue λ_2.

(b) *Connection of two vertices of the same graph.* Let v_{I} be a vector having $+1$ in the i-th component, -1 in the j-th component and zeros otherwise, and let $u_{\mathrm{I}}(t)$ be the function belonging to this starting-vector. For all starting-vectors of this kind we have $\bar{u}=0$. So we can interprete $u_{\mathrm{I}}(t)$ as a transportation of one unit of liquid from x_i to x_j. With v_{II} having $+1$ in the k-th component and -1 in the l-th one and zeros otherwise we start an analogous transportation $u_{\mathrm{II}}(t)$ from x_k to x_l. We call the pair of vertices x_i, x_j better connected than the pair x_k, x_l, if there is a time t_0 such that for all $t>t_0$ we have $\|u_{\mathrm{I}}(t)\|_2<\|u_{\mathrm{II}}(t)\|_2$.

Lemma 3.1. *Let λ_2 be an r-fold eigenvalue and let $u^{(2,1)},\dots,u^{(2,r)}$ denote corresponding orthonormal eigenvectors. If*

$$\left(\sum_{s=1}^{r}(u^{(2,s)},v_{\mathrm{I}})^2\right)^{1/2}<\left(\sum_{s=1}^{r}(u^{(2,s)},v_{\mathrm{II}})^2\right)^{1/2},$$

then x_i, x_j are better connected than x_k, x_l. (N.B. This condition means that the portion of v_{I} lying in the eigenspace of λ_2 is smaller than in the case of v_{II}.)

Proof. We have

$$\begin{aligned}\|u_{\mathrm{I}}(t)\|_2&=\left(\left(\sum_{s=1}^{r}(u^{(2,s)},v_{\mathrm{I}})^2\right)\mathrm{e}^{-2kt}\varphi_2^2(t)+\sum_{s=r+2}^{n}(u^{(s)},v_{\mathrm{I}})^2\mathrm{e}^{-2kt}\varphi_s^2(t)\right)^{1/2}\\&=\left(\sum_{s=1}^{r}(u^{(2,s)},v_{\mathrm{I}})^2+\sum_{s=r+2}^{n}(u^{(s)},v_{\mathrm{I}})^2\left[\frac{\varphi_s(t)}{\varphi_2(t)}\right]^2\right)^{1/2}\cdot\mathrm{e}^{-kt}\varphi_2(t)\end{aligned}$$

with $\lim_{t\to\infty}\varphi_s(t)/\varphi_2(t)=0$. An analogous expression holds for $\|u_{\mathrm{II}}(t)\|_2$. If the assumption of the lemma holds, we thus have $\exists t_0$: $\forall t>t_0$:

$$\begin{aligned}\mathrm{e}^{kt}\varphi_2^{-1}(t)\cdot\|u_{\mathrm{I}}(t)\|_2&=\left(\sum_{s=1}^{r}(u^{(2,s)},v_{\mathrm{I}})^2+\sum_{s=r+2}^{n}(u^{(s)},v_{\mathrm{I}})^2\left[\frac{\varphi_s(t)}{\varphi_2(t)}\right]^2\right)^{1/2},\\&<\left(\sum_{s=1}^{r}(u^{(2,s)},v_{\mathrm{II}})^2+\sum_{s=r+2}^{n}(u^{(s)},v_{\mathrm{II}})^2\left[\frac{\varphi_s(t)}{\varphi_2(t)}\right]^2\right)^{1/2}\\&=\mathrm{e}^{kt}\cdot\varphi_2^{-1}(t)\cdot\|u_{\mathrm{II}}(t)\|_2.\end{aligned}$$

As $\mathrm{e}^{kt}\varphi_2^{-1}(t)$ is strictly positive, the lemma is proven.

(c) *Position of a vertex.* Let v_{I} be a vector having $+1$ in the i-th component and zero otherwise and let $u_{\mathrm{I}}(t)$ be the corresponding solution of (2.1). Let v_{II} have $+1$ only in its j-th component and let $u_{\mathrm{II}}(t)$ be the solution of (2.1) with starting-vector v_{II}. For $\bar{u} := (1/n)(1, \dots, 1)^{\mathrm{T}}$ we have $\lim_{t\to\infty} u_{\mathrm{I}}(t) = \bar{u} = \lim_{t\to\infty} u_{\mathrm{II}}(t)$. We say that x_i has a better position in the graph than x_j, if there exists a time t_0 such that for all $t > t_0$ we have $\|u_{\mathrm{I}}(t) - \bar{u}\|_2 < \|u_{\mathrm{II}}(t) - \bar{u}\|_2$.

Lemma 3.2. *If*

$$\left(\sum_{s=1}^{r} (u^{(2,s)}, v_{\mathrm{I}})^2\right)^{1/2} < \left(\sum_{s=1}^{r} (u^{(2,s)}, v_{\mathrm{II}})^2\right)^{1/2},$$

then x_i has a better position than x_j.

Proof. Analogous to the proof of Lemma 3.1.

Examples. We shall apply our definitions and results to the two graphs shown in Fig. 1. Their spectra are:

G_1: $\lambda_1 = 0$ $\quad u^{(1)} = \dfrac{1}{\sqrt{5}}(1,1,1,1,1)^{\mathrm{T}}$

$$\lambda_2 = \frac{1}{2}(\sqrt{5}-3) \qquad u^{(2)} = \frac{1}{2}\left(\sqrt{1+\frac{1}{\sqrt{5}}}, \sqrt{1-\frac{1}{\sqrt{5}}}, 0, -\sqrt{1-\frac{1}{\sqrt{5}}}, -\sqrt{1+\frac{1}{\sqrt{5}}}\right)^{\mathrm{T}}$$

$$\lambda_3 = \frac{1}{2}(\sqrt{5}-5) \qquad u^{(3)} = \frac{1}{\sqrt{40}}(-\sqrt{5}-1, \sqrt{5}-1, 4, \sqrt{5}-1, -\sqrt{5}-1)^{\mathrm{T}}$$

$$\lambda_4 = \frac{1}{2}(-\sqrt{5}-3) \qquad u^{(4)} = \frac{1}{2}\left(\sqrt{1-\frac{1}{\sqrt{5}}}, -\sqrt{1+\frac{1}{\sqrt{5}}}, 0, \sqrt{1+\frac{1}{\sqrt{5}}}, -\sqrt{1-\frac{1}{\sqrt{5}}}\right)^{\mathrm{T}}$$

$$\lambda_5 = \frac{1}{2}(-\sqrt{5}-5) \qquad u^{(5)} = \frac{1}{\sqrt{40}}(\sqrt{5}-1, -\sqrt{5}-1, 4, -\sqrt{5}-1, \sqrt{5}-1)^{\mathrm{T}}$$

G_2: $\lambda_1 = 0$ $\quad u^{(1)} = \dfrac{1}{\sqrt{5}}(1,1,1,1,1)^{\mathrm{T}}$

$$\lambda_2 = -1 \qquad u^{(2)} = \frac{1}{\sqrt{2}}(1,0,0,0,-1)^{\mathrm{T}}$$

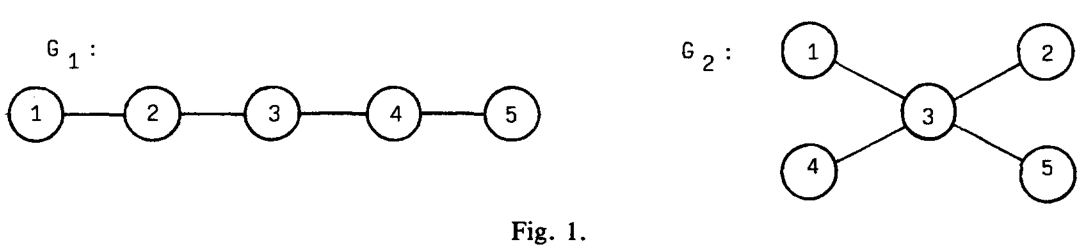


Fig. 1.

$$\lambda_3=-1 \qquad u^{(3)}=\frac{1}{2}(1,-1,0,-1,1)^{\mathrm{T}}$$

$$\lambda_4=-1 \qquad u^{(4)}=\frac{1}{\sqrt{2}}(0,1,0,-1,0)^{\mathrm{T}}$$

$$\lambda_5=-5 \qquad u^{(5)}=\frac{1}{\sqrt{20}}(-1,-1,4,-1,-1)^{\mathrm{T}}$$

If the liquid we fill the pipes with is chosen such that $k\in(0,\sqrt{0.382})$, $u(t)$ is a sum of vibrations in both graphs. For every $k\in(\sqrt{0.382},\sqrt{5})$ there are starting vectors v for which $u(t)$ is a sum of periodic functions in G_2 but not in G_1. For $k>\sqrt{5}$, $u(t)$ is a sum of decaying exponential functions in both graphs. For e.g. $k=2.5$ we have as half-life in G_1 $\tau_1=4.39$ and G_2 $\tau_2=3.32$, so G_1 is less permeable than G_2, a result which certainly corresponds to our intuitive notion of permeability. Starting with $v=(1.203,0.7435,0,0.7435,-1.203)^{\mathrm{T}}$, which is an eigenvector for both graphs, and calling the solution of (2.1) $u_{\mathrm{I}}(t)$ for G_1 and $u_{\mathrm{II}}(t)$ for G_2 we get

t	$\lVert u_{\mathrm{I}}(t)\rVert_2$	$\lVert u_{\mathrm{II}}(t)\rVert_2$
0	2	2
2	1.508	1.377
4	1.100	0.907
6	0.802	0.598
8	0.585	0.394
10	0.426	0.250
20	0.088	0.032

So the convergence towards $\bar{u}=0$ is indeed significantly slower in G_1 than in G_2. Taking into account the symmetries in the graphs we have 6 different pairs of vertices in G_1 and two in G_2. As λ_2 in G_1 is a simple eigenvalue, we only have to consider the scalar product $|(u^{(2)},v)|$. For the well-connectedness of pairs of vertices we thus get:

in G_1:

vertices	$\lvert(u^{(2)},v)\rvert$
x_1,x_5	$\sqrt{1+\frac{1}{\sqrt{5}}}=1.203$
x_1,x_4	$\frac{1}{2}\left(\sqrt{1+\frac{1}{\sqrt{5}}}+\sqrt{1-\frac{1}{\sqrt{5}}}\right)=0.9732$
x_2,x_4	$\sqrt{1-\frac{1}{\sqrt{5}}}=0.7435$
x_1,x_3	$\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{5}}}=0.6015$
x_2,x_3	$\frac{1}{2}\sqrt{1-\frac{1}{\sqrt{5}}}=0.3718$
x_1,x_2	$\frac{1}{2}\left(\sqrt{1+\frac{1}{\sqrt{5}}}+\sqrt{1-\frac{1}{\sqrt{5}}}\right)=0.2298$

in G_2:

vertices	$\left(\sum_{s=2}^{4}(u^{(s)},v)^2\right)^{1/2}$
x_1,x_2	$\sqrt{2}$
x_1,x_3	$\frac{1}{2}\sqrt{3}$

The results for G_2 certainly do not surprise us very much. In G_1 we would perhaps not have expected that x_1 and x_3 are better connected than x_2, x_4. This is likely to stem from the fact that during the transport between x_1 and x_3 only at the vertex x_3 some liquid can go 'wrong', i.e., flow to x_4 or x_5. (A similar argument should hold for the pair x_1, x_2 compared to x_2, x_3.)

When investigating the position of the vertices, we have to distinguish three cases in G_1 and again two in G_2:

in G_1:

vertex	$\lvert(u^{(2)}, v)\rvert$
x_1	$\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{5}}}$
x_2	$\frac{1}{2}\sqrt{1-\frac{1}{\sqrt{5}}}$
x_3	0

in G_2:

vertex	$\left(\sum_{s=2}^{4} (u^{(s)}, v)^2\right)^{1/2}$
x_1	$\frac{1}{2}\sqrt{3}$
x_3	0

Up to now the terms permeability, connection and position have been apparently unrelated. In the following section we shall investigate how we can change the permeability of a graph by inserting a new edge and we shall find that it is feasible to expect that a new edge in a connected graph will improve the permeability the more the worse connected it endvertices are up to now and that it is a good way of connecting two components of a graph when we take the vertices with the best position in each one of the components as endvertices of the linking edge.

4. The result of inserting an edge

If we insert and edge $x_i x_j$ into the graph G, this results in a change of its admittance matrix D that can be described by the addition of a matrix B which (after some simultaneous permutations of columns and rows) has the form

$$\begin{pmatrix} -1 & 1 & 0 & \dots & 0 \\ 1 & -1 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & 0 \end{pmatrix}$$

So B is negative semidefinite and has rank one. Thus for the spectrum $\mu_1, \dots, \mu_n$ of $D+B$ we have $0=\lambda_1=\mu_1 \ge \lambda_2 \ge \mu_2 \ge \lambda_3 \ge \dots \ge \lambda_n \ge \mu_n$ (cf. [2, Theorem 2.1]). This means that by inserting an edge the permeability of the graph cannot become worse. If λ_2 is a multiple eigenvalue, we have $\lambda_2 = \mu_2$ (with their multiplicities differing by at most one), and if λ_2 is a simple eigenvalue, it can happen that $\lambda_2 > \mu_2$, i.e., the permeability is improved strictly. An example for the fact that the latter need not

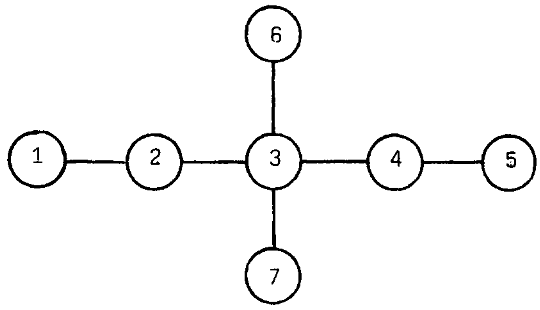


Fig. 2.

happen is the graph shown in Fig. 2 the second eigenvalue of which remains $\lambda_2 = -0.38197 = \mu_2$ no matter whether there is an edge x_6x_7 or not (though this edge influences one higher eigenvalue).

Of course it would be highly desirable to compute the eigenvalues and eigenvectors of $D+B$ directly from those of D and B. As this is impossible in general, in the sequel we shall derive upper and lower bounds for μ_2 so that we shall be able to estimate which choice of endvertices for a new edge will result in small or large changes of the permeability. The vertices to be connected by the new edge are called x_i and x_j. With v being defined as a vector with $+1$ with the i-th component and -1 in the j-th one and zero otherwise we have $B = -vv^{\mathrm{T}}$, and finally we define $\alpha := |(v, u^{(2)})| = |u_i^{(2)} - u_j^{(2)}|$.

4.1. The case of connected graphs

(In this subsection we assume λ_2 to be simple.) It is rather easy to give a lower bound for μ_2 (i.e., an expression giving the maximal possible change of the permeability). For every vector $w \perp u^{(1)}$ (the latter remains an eigenvector of $D+B$) the Rayleigh quotient of w has this property. Let us particularly consider $w = u^{(2)}$. We have

$$R(u^{(2)}) = u^{(2)\mathrm{T}}(D+B)u^{(2)} = \lambda_2 - u^{(2)\mathrm{T}}vv^{\mathrm{T}}u^{(2)} = \lambda_2 - \alpha^2.$$

This expression is the lower the higher α^2 is (i.e., the worse connected x_i and x_j are). Together with the previous considerations we have

$$\mu_2 \geq \max\{\lambda_2 - \alpha^2, \lambda_3\}. \tag{4.1}$$

For the construction of an upper bound for μ_2 (i.e., an expression giving the minimally possible change of the permeability) we shall use the technique of intermediate eigenvalue problems. To be conform with the presentation in [7] we shall now look for a lower bound for the least but one eigenvalue of $-D + vv^{\mathrm{T}}$. To make the second matrix in the sum positive definite, we replace it by $C := vv^{\mathrm{T}} + \varepsilon I$, $\varepsilon > 0$. With $k = 2$, $p^{(r)} := C^{-1}u^{(r)}$, $r = 1, \ldots, k$ we get the matrix

$$(\gamma_{rs})_{r,s=1,2} := ((p^{(r)}, Cp^{(s)}))^{-1}_{r,s=1,2} = \begin{pmatrix} \varepsilon & 0 \\ 0 & \dfrac{\varepsilon}{1+\dfrac{1}{2+\varepsilon}\alpha^2} \end{pmatrix}$$

Our intermediate problem then reads

$$-Du + (u, u^{(1)})\gamma_{11}u^{(1)} + (u, u^{(2)})\gamma_{22}u^{(2)} = \nu u.$$

Its spectrum is

$$\nu_1 = \varepsilon, \quad \nu_2 = -\lambda_2 + \frac{\varepsilon}{1+\dfrac{1}{2+\varepsilon}\alpha^2}, \nu_3 = -\lambda_3, \ldots, \nu_n = -\lambda_n.$$

The value we are looking for is the second largest one in this sequence. If $\varepsilon < \nu_3$, it is $\min\{\nu_2, \nu_3\}$. The upper bound for μ_2 is then

$$\mu_2 \leq \max\{-\nu_2 + \varepsilon, -\nu_3 + \varepsilon\} = \max\left\{\lambda_2 - \frac{\varepsilon\alpha^2}{\varepsilon + (2-\alpha^2)}, \lambda_3 + \varepsilon\right\}. \tag{4.2}$$

As the first term decreases with increasing ε whereas the second one increases, the best upper bound is achieved by a choice of ε that makes both terms equal. For $\beta := \lambda_2 - \lambda_3$ we let

$$\varepsilon := \frac{\beta-2}{2} + \left(\frac{(\beta-2)^2}{4} + \beta(2-\alpha^2)\right)^{1/2}.$$

The higher α^2 is the lower is ε and the lower is the upper bound. In the extreme we have

$$\alpha^2 = 0 \Rightarrow \varepsilon = \lambda_2 - \lambda_3 \Rightarrow \mu_2 = \lambda_2,$$

$$\alpha^2 = 2 \Rightarrow \begin{cases} \varepsilon = \lambda_2 - \lambda_3 - 2 \\ \nu_2 > \nu_3 \quad \forall \varepsilon > 0 \end{cases} \Rightarrow \mu_2 = \begin{cases} \lambda_2 - 2 & \text{if } \beta - 2 \geq 0, \\ \lambda_3 & \text{if } \beta - 2 < 0 \end{cases}$$

(the equality signs for μ_2 hold because of the lower bound).

So these bounds indicate that the change in the graph's permeability should be the larger the worse connected the endvertices of the new edge are.

Example. Let us once again consider the path with 5 vertices shown in Fig. 1. We compare the effect of inserting four different edges alternatively:

endvertices	lower bound	μ_2	upper bound
x_1x_5	−1.3820	−1.3820	−0.9860
x_1x_4	−1.3292	−0.8299	−0.7406
x_2x_4	−0.9348	−0.6972	−0.5792
x_1x_3	−0.7438	−0.5188	−0.5078
none	–	−0.3820	–

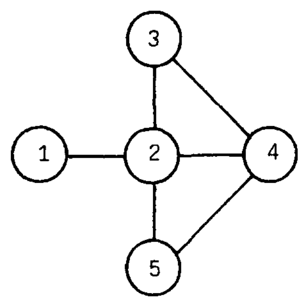


Fig. 3.

We see that the expected effect indeed occurs. Unfortunately, the intervals we get for μ_2 are not all pairwise disjoint, so this leaves open the possibility that there are graphs for which the insertion of a certain edge yields a lower μ_2 than another one although its endvertices are already better connected than the other one's. The inverse of our expected relationship is not true, anyway: if an edge yields a lower second eigenvalue than another one, its endvertices need not have a larger α^2 than the other one's. As an example take the graph shown in Fig. 3. The second eigenvector is $u^{(2)}=(1/\sqrt{12})(-3;0;1;1;1)^{\mathrm{T}}$ with $\lambda_2=-1$, and the edge x_1x_4 yields $\mu_2=-2$, whereas for x_1x_3 we only get $\mu_2=-3+\sqrt{2}=-1.5858$.

4.2. *Connecting two components*

If G has two components of m and $n-m$ vertices respectively, its spectrum is the union of the spectra of the components. Zero is a double eigenvalue for which we take as eigenvectors

$$u^{(1)}=\frac{1}{\sqrt{n}}(1,\dots,1)^{\mathrm{T}},$$

$$u^{(2)}=\frac{1}{\sqrt{nm(n-m)}}(n-m,\dots,n-m,-m,\dots,-m)^{\mathrm{T}}$$

(thus $v^{(1)}$ remains an eigenvector even after adding an edge). The third largest eigenvalue λ_3 is the second largest eigenvalue of one of the components, without loss of generality let it be the component with vertices $x_1,\dots,x_m$. For the sake of easier reference let $\lambda_5,\lambda_7,\dots,\lambda_{2m-1}$ be the other eigenvalues of this component and let $\lambda_4,\lambda_6,\dots,\lambda_{2(n-m)}$ be the other one's spectrum (so λ_4 need not be the fourth largest eigenvalue, e.g., if one component is a path of length m and the other one is the complete graph K_m, then λ_4 is in fact the $(m+2)$-nd largest eigenvalue). Even if the components have some eigenvalues in common, we shall assume the eigenvectors to be of the form

$$u^{(i)}=\begin{cases}(u_1^{(i)},\dots,u_m^{(i)},0,\dots,0)^{\mathrm{T}}, & \text{if } i \text{ is odd},\\ (0,\dots,0,u_{m+1}^{(i)},\dots,u_n^{(i)})^{\mathrm{T}}, & \text{if } i \text{ is even}.\end{cases}$$

If a new edge is inserted into one of the components, the second eigenvalue of the graph remains zero. If a new edge links both components it decreases strictly. In this case, we shall again try to derive bounds for the new second eigenvalue μ_2 which this time are intended to support the idea that the largest improvement of the permeability occurs when we take the vertices with the best position in the respective components as endvertices for the new edge. In principle, we shall use the same techniques as above, but things are much more difficult now, because we must draw conclusions about μ_2 not from λ_2 but from λ_3 and λ_4, i.e., from eigenvalues that can be very far away from the interval we want to describe. If e.g. we just compute the Rayleigh quotient for $u^{(2)}$, we get

$$\mu_2 \geq \frac{-n}{m(n-m)} =: -\psi. \tag{4.3}$$

This is not an unimportant result, because it says that by linking two components each of which has at least two vertices, for $n>4$ (the case of $n=4$ can be established by direct computation) we can never reach $\mu_2=-1$, but it gives no information whatsoever about which vertices we should choose. In order to get a more detailed lower bound we have to look for a linear combination of $u^{(2)}, u^{(3)}, u^{(4)}$ the Rayleigh quotient of which looks useful. To this purpose we project the eigenvalue problem onto $\mathrm{span}\{u^{(1)}, \ldots, u^{(4)}\}$ thus getting the problem

$$Mw = \nu N w$$

with $M=(u^{(k)\mathrm{T}}(D+B)u^{(l)})_{k,l=1,\ldots,4}$, $N=(u^{(k)\mathrm{T}}u^{(l)})_{k,l=1,\ldots,4}=I$.

Let $u_i^{(3)}=a$, $u_j^{(4)}=b$; we then have

$$M=\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -\psi & -\sqrt{\psi}a & \sqrt{\psi}b \\ 0 & -\sqrt{\psi}a & \lambda_3-a^2 & ab \\ 0 & \sqrt{\psi}b & ab & \lambda_4-b^2 \end{pmatrix}.$$

Leaving aside the first row and column belonging to $\nu_1=\mu_1=\lambda_1=0$ we have to find the roots of the characteristic polynomial of the remaining submatrix. It reads:

$$\begin{aligned} p(\nu) = {} & -\nu^3 + (-\psi+\lambda_3+\lambda_4-a^2-b^2)\nu^2 \\ & -(\lambda_3\lambda_4-\lambda_3(\psi+b^2)-\lambda_4(\psi+a^2))\nu-\lambda_3\lambda_4\psi. \end{aligned} \tag{4.4}$$

We have

$$p(0) = -\lambda_3\lambda_4\psi < 0,$$

$$p(\lambda_3) \geq 0 \qquad (p(-\psi)\geq 0, \text{ if } \psi \leq |\lambda_3|),$$

$$p(\lambda_4) \leq 0,$$

$$\lim_{\nu\to-\infty} p(\nu) = \infty.$$

We call the greatest root of $p(\nu)$ ν_2 and can state that it must be in the interval

$]\max\{\lambda_3, -\psi\}, 0[$ so that ν_2 (which can be determined numerically) itself is a better bound than $-\psi$. Let $\hat{p}(\nu)$ contain all terms of p that are independent of a^2 and b^2. We than have

$$p(\nu) = \hat{p}(\nu) - \nu(b^2(\nu - \lambda_3) + a^2(\nu - \lambda_4)).$$

So for all $\nu \in]\lambda_3, 0[$ $p(\nu)$ is the greater the greater $a^2 + b^2$ is. As $p(\nu)$ is monotonically decreasing in a nonempty interval containing ν_2, this relationship must also hold for the dependence of ν_2 from $a^2 + b^2$. So, if we connect two coponents via two vertices with a bad position, we get a lower bound for μ_2 that forbids a high permeability for the new graph whereas if we let the 'bridge' run between two well positioned vertices, ν_2 allows μ_2 to be small.

During the establishment of the lower bound we already had to use indirect arguments to some extent. This can be avoided even less while deriving an expression for an upper bound. Like before, we try to approximate the second lowest eigenvalue of $-D + (vv^{\mathrm{T}} + \varepsilon I)$ $(=: -D + C)$ from below by the solutions of an intermediate eigenvalue problem; only this time we have to use four vectors

$$p^{(1)} := C^{-1}u^{(1)}, \ldots, p^{(4)} := C^{-1}u^{(4)}.$$

The matrix $(\gamma_{kl})_{k,l=1,\ldots,4}$ is again defined as $((p^{(k)}, Cp^{(l)}))^{-1}_{k,l=1,\ldots,4}$. The intermediate problem then reads

$$-Du + \sum_{k=1}^{4} \sum_{l=1}^{4} (u, u^{(k)}) \gamma_{kl} u^{(l)} = \nu u.$$

Its spectrum is

$$\begin{array}{ll} \nu_1 = \varepsilon & \text{with eigenvector } u^{(1)}, \\ \nu_5 = -\lambda_5 & \text{with eigenvector } u^{(5)}, \\ \ldots & \ldots \\ \nu_n = -\lambda_n & \text{with eigenvector } u^{(n)}. \end{array}$$

The missing eigenvalues form the spectrum of the matrix

$$\begin{pmatrix} -\lambda_2 + \gamma_{22} & \gamma_{23} & \gamma_{24} \\ \gamma_{23} & -\lambda_3 + \gamma_{33} & \gamma_{34} \\ \gamma_{24} & \gamma_{34} & -\lambda_4 + \gamma_{44} \end{pmatrix}.$$

If we compute the explicit values of the numbers γ_{kl}, there remains the task of evaluating the characteristic polynomial (with $N := 2 + \varepsilon - \psi - a^2 - b^2$):

$$p(\nu) = \det \begin{pmatrix} \dfrac{(N+\psi)\varepsilon}{N} - \nu & \dfrac{a\sqrt{\psi}\varepsilon}{N} & \dfrac{-b\sqrt{\psi}\varepsilon}{N} \\ \dfrac{a\sqrt{\psi}\varepsilon}{N} & \dfrac{(N+a^2)\varepsilon}{N} - \lambda_3 - \nu & \dfrac{-ab\varepsilon}{N} \\ \dfrac{-b\sqrt{\psi}\varepsilon}{N} & \dfrac{-ab\varepsilon}{N} & \dfrac{(N+b^2)\varepsilon}{N} - \lambda_4 - \nu \end{pmatrix}$$

which can also be written in the form

$$p(\nu)=\frac{1}{N}\{[(2+\varepsilon)(\varepsilon-\nu)+\psi\nu](-\nu-\lambda_4+\varepsilon)(-\nu-\lambda_3+\varepsilon)$$
$$-a^2(-\nu-\lambda_4+\varepsilon)(-\lambda_3-\nu)(\varepsilon-\nu)$$
$$-b^2(-\nu-\lambda_3+\varepsilon)(-\lambda_4-\nu)(\varepsilon-\nu)\}. \tag{4.5}$$

Again we can localize its roots ν_2, ν_3, ν_4 by the following considerations

$$p(\varepsilon)=\lambda_3\lambda_4\psi\frac{\varepsilon}{N}>0 \quad (\text{if } \varepsilon\neq 0),$$

$$p(-\lambda_3+\varepsilon)=\frac{\varepsilon}{N}(\lambda_3-\lambda_4)a^2\lambda_3<0 \quad (\text{if } \lambda_3\neq\lambda_4 \text{ and } a^2\neq 0),$$

$$p(-\lambda_4+\varepsilon)=\frac{\varepsilon}{N}(\lambda_4-\lambda_3)b^2\lambda_4>0 \quad (\text{if } \lambda_3\neq\lambda_4 \text{ and } b^2\neq 0),$$

$$\lim_{\nu\to\infty} p(\nu)=-\infty.$$

So we have $\nu_2\in\,]\varepsilon,-\lambda_3+\varepsilon[$ and if $\nu_2\leq\min\{\nu_5,\nu_6\}$ $(=-\max\{\lambda_5,\lambda_6\})$, an upper bound for μ_2 is

$$\mu_2\leq-\nu_2+\varepsilon.$$

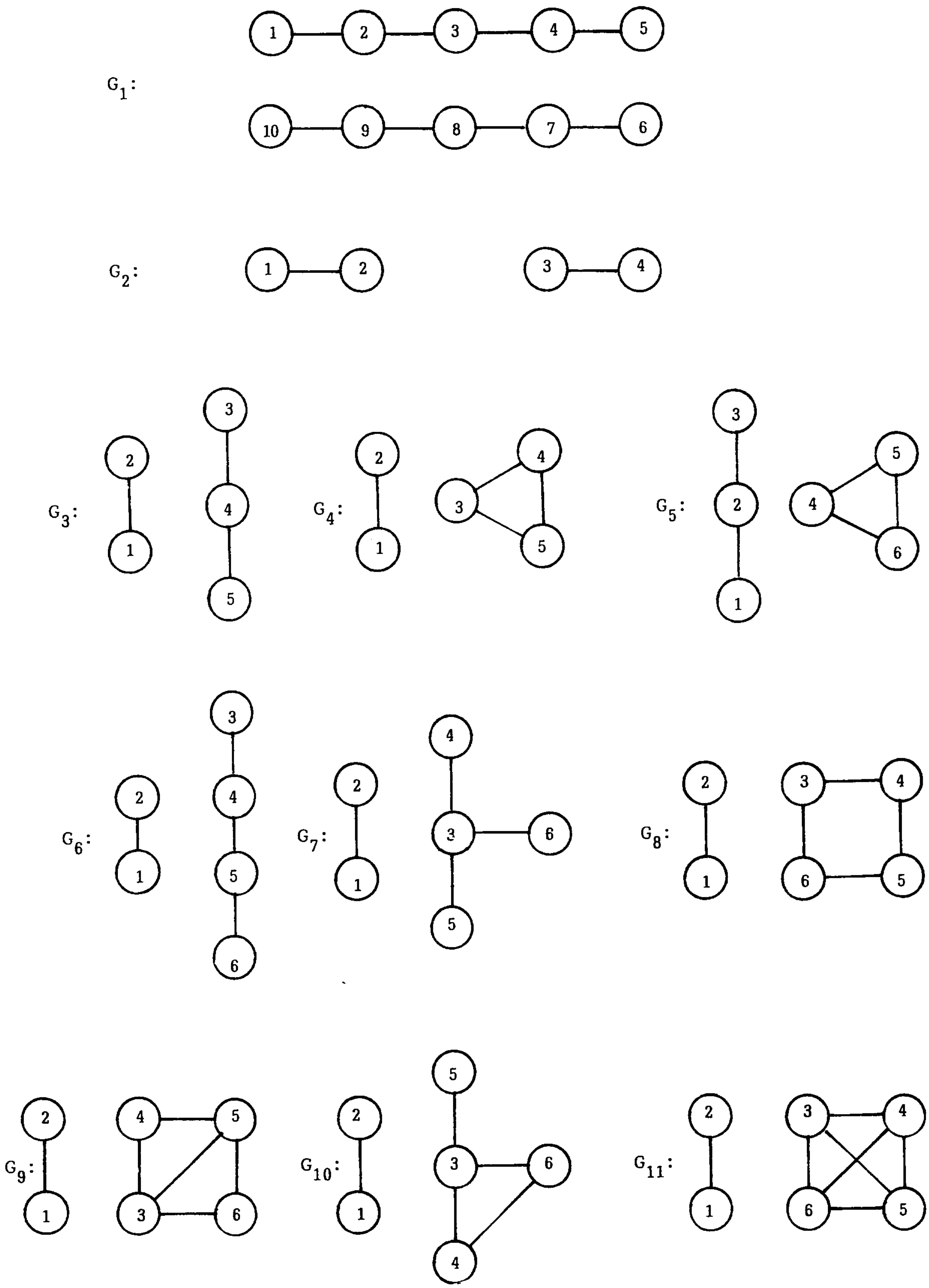
Our aim should now be to establish that this bound rises with rising a^2+b^2, but this in fact does only hold under special circumstances: As this does not influence the position of the roots, we shall now investigate the polynomial $\bar{p}(\nu):=N\cdot p(\nu)$. For $a^2+b^2=0$ its roots are

$$\nu_2=\frac{\varepsilon(2+\varepsilon)}{2+\varepsilon-\psi}, \qquad \nu_3=-\lambda_3+\varepsilon, \qquad \nu_4=-\lambda_4+\varepsilon.$$

To make a fixed number $\hat{\nu}$ the smallest positive root of $\bar{p}$ (with positive ε) it is necessary and sufficient to let

$$\varepsilon:=\frac{\hat{\nu}-2}{2}+\sqrt{\frac{(\hat{\nu}+2)^2}{4}-\psi\hat{\nu}}.$$

There is a neighbourhood of $\hat{\nu}$ in which $\bar{p}$ is strictly monotonely decreasing. Let us now increase a^2 and b^2 (leaving ε constant). If $\hat{\nu}>-\lambda_3$, there is a neighbourhood of $\hat{\nu}$ in which $\bar{p}(\nu)$ decreases with increasing a^2. Thus the root ν_2 becomes less than $\hat{\nu}$ and decreases with increasing a^2. As ε is kept constant, the upper bound for μ_2 increases, i.e., the increase in permeability we can guarantee is reduced. An analogous statement holds for b^2, if $\hat{\nu}>-\lambda_4$. As we must not increase ν_2 beyond $\min\{-\lambda_5,-\lambda_6\}$, the bound moves completely as intended only if $\lambda_5<\lambda_4$ and $\lambda_6\neq\lambda_4$. If $\lambda_4<\lambda_5<\lambda_3$, we still have the desired result for the choice of the endvertex in the less permeable component. (For $\lambda_5=\lambda_3$ or $\lambda_6=\lambda_4$ we could not expect much any-



G1:
1
2
3
4
5
10
9
8
7
6
G2:
1
2
3
4
G3:
2
1
3
4
5
G4:
2
1
4
3
5
G5:
3
2
1
5
4
6
G6:
2
1
3
4
5
6
G7:
2
1
4
3
6
5
G8:
2
1
3
4
6
5
G9:
2
1
4
5
3
6
G10:
2
1
5
3
6
4
G11:
2
1
3
4
6
5

Fig. 4.

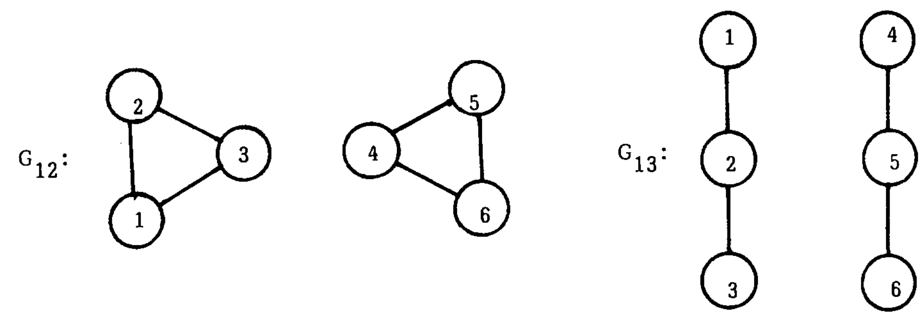


Fig. 4 (contd.).

way, because then for an arbitrary vertex in the respective component there is always an eigenvector having zero in the corresponding entry no matter what position this vertex really has. This was no problem for the lower bound, because in order to make the bound as tight as possible we have to choose the eigenvector with the highest possible entry for the vertex in question in the case of λ_3 or λ_4 being a multiple eigenvalue.)

Examples. First of all let us examine a graph G_1 consisting of two paths of length five. See Fig. 4. Here are six different possibilities for linking the two components by an edge. Since $\lambda_3=\lambda_4=-0.38197$ and $\lambda_5=\lambda_6=-1.38197$, we can expect that our upper and lower bounds will be the lower the better the position of the endvertices of the new edge are. This is indeed the case, although as in the previous subsection the intervals we get are not always disjoint

endvertices	lower bound	μ_2	upper bound
x_3x_8	-0.3820	-0.2087	-0.1718
x_3x_9	-0.2174	-0.1700	-0.1443
x_4x_9	-0.1725	-0.1487	-0.1273
x_3x_{10}	-0.1544	-0.1277	-0.1192
x_4x_{10}	-0.1330	-0.1172	-0.1080
x_5x_{10}	-0.1094	-0.0979	-0.0953

To give an idea about what results one can still get with our methods, if $\mu_2 \gg \lambda_3$, let us link two copies of the complete graph K_5 by an edge. We have $\lambda_1=\lambda_2=0$, $\lambda_3=\cdots=\lambda_{10}=-5$. For the permeability of the new graph we get:

lower bound: -0.3295,
μ_2: -0.2984,
upper bound: -0.2984.

We conclude the examples' section with a list of all graphs with not more than six vertices and two nontrivial components.

graph	insert edge	lower bound	μ_2	upper bound
G_2	x_2x_3	−0.5858	−0.5858	−0.5858
G_3	x_2x_3	−0.3909	−0.3820	−0.3820
	x_2x_4	−0.6126	−0.5188	−0.5188
G_4	x_2x_3	−0.5392	−0.5188	−0.5188
G_5	x_2x_4	−0.5535	−0.4384	−0.4384
	x_3x_4	−0.3422	−0.3249	−0.3249
G_6	x_2x_3	−0.2795	−0.2680	−0.2667
	x_2x_4	−0.4239	−0.3820	−0.3655
G_7	x_2x_3	−0.5570	−0.4859	−0.3139
	x_2x_4	−0.3596	−0.3249	−0.3139
G_8	x_2x_3	−0.4553	−0.4384	−0.4189
G_9	x_2x_3	−0.5570	−0.4859	−0.4859
	x_2x_4	−0.4553	−0.4384	−0.4384
G_{10}	x_2x_3	−0.5570	−0.4859	−0.4627
	x_2x_4	−0.4594	−0.4131	−0.4114
	x_2x_5	−0.3275	−0.3249	−0.3239
G_{11}	x_2x_3	−0.5074	−0.4859	−0.4859
G_{12}	x_3x_4	−0.4774	−0.4384	−0.4384
G_{13}	x_2x_5	−0.6667	−0.4384	−0.4384
	x_2x_4	−0.3713	−0.3249	−0.3249
	x_1x_4	−0.2792	−0.2680	−0.2680

5. The sequence of spectra during the construction of a graph

When a graph is constructed from the empty graph by a sequential insertion of edges, one in general has the choice between several sequences of subgraphs occurring during this construction. Among these are sequences that are characterized by the fact that the corresponding sequence of spectra fulfils certain optimality conditions. The following two examples are meant to illustrate the questions:

(i) Which sequence of subgraphs we get when imposing certain conditions on the occurring spectra, and

(ii) What kinds of conditions we must impose in order to get a certain sequence of subgraphs.

5.1. Subgraphs resulting from spectral conditions

The complete graph K_n shall be constructed in such a way that the permeability changes after the insertion of as few edges as possible and that this change, whenever it occurs, shall be as large as possible.

The main part of the solution of this problem by the following observation:

Lemma 5.1. *The star $K_{1,n-1}$ is the most permeable tree with n vertices.*

Proof. (As all trees with at most 3 vertices are stars, we shall now assume $n \geq 4$.)

A star has the spectrum $\lambda_1=0$, $\lambda_2=\cdots=\lambda_{n-1}=-1$, $\lambda_n=-n$. If a tree is not a star, it must have at least two vertices of degree at least two. Deleting an arbitrary edge on the path between these two vertices yields exactly two components each with at least two vertices. If both components are isomorphic to K_2, the original tree was a path of length four and thus had as second eigenvalue $\lambda_2=-2+\sqrt{2}>-1$, otherwise we can see from (4.3) that linking the components again by any edge (in particular by the one just deleted) must yield a second eigenvalue strictly greater than -1.

Now we can construct the feasible sequence of subgraphs:

(i) As for the empty graph zero is an n-fold eigenvalue, the permeability can only change after the insertion of $n-1$ edges, if they are used to construct a spanning tree. The best permeability is achieved, if this tree is isomorphic to $K_{1,n-1}$ (w.l.o.g. let x_n be the 'center').

(ii) For $i=1,\ldots,n-2$ let H_i be a graph with the following characteristics:

(α) The vertices $x_{n-i+1},\ldots,x_n$ form a complete subgraph.

(β) The vertices $x_1,\ldots,x_{n-i}$ form an empty subgraph.

(γ) All edges x_kx_l with $k\leq n-i$, $l\geq n-i+1$ exist.

(In particular: $H_1\cong K_{1,n-1}$.)

As $-i$ is an $n-(i+1)$-fold eigenvalue, the permeability can only change after the insertion of $n-(i+1)$ edges, if they are used to construct a spanning tree for the vertex set $\{x_1,\ldots,x_{n-i}\}$. The best permeability is achieved, if this tree is isomorphic to $K_{1,n-i}$ (w.l.o.g. let x_{n-i} be the 'center'). The resulting graph is H_{i+1}.

(iii) For $i=n-1$ we have $H_i\cong K_n$.

The graphs H_i, $i<n-1$ have a remarkably property. Not only do they have diameter two (which is optimal for noncomplete graphs) and connectivity i, but between every pair of vertices there are i disjoint paths of length at most two.

5.2. Spectral conditions resulting from sequences of subgraphs

During the construction of a path with n vertices we want the occurring subgraphs to be paths with k vertices plus $n-k$ isolated vertices. Then we should impose the condition that every new edge should change as many eigenvalues as possible. From the second edge onwards the linking of two isolated vertices via a new edge only changes one eigenvalue from 0 to -2, whereas the extension of an existing path by one vertex changes at least one zero eigenvalue and the lowest eigenvalue of the path.

If on the other hand we want our construction to produce initially as many copies of K_2 as possible and to join them to paths of greater lengths afterwards, we should demand that the first nonzero eigenvalue should become as low as possible (this is due to the fact that joining two components with at least two vertices always yields a permeability of the new component that is worse than the permeability of each one of the original components. Therefore the edges have to be used for the construction of as many short paths as possible.)

5.3. *Comparison with $\varrho(A)$*

In the papers mentioned in the introduction the spectral radius $\varrho(A)$ of the adjacency matrix A of a graph was introduced as a measure of quality for a graph, similar to what we have done here with the notion of permeability. Since one can see that the maximal clique size of G is a lower bound for $\varrho(A)$ (e.g. from [6, Theorem 2.1]), while $-\lambda_2$ can never exceed the (vertex-) connectivity of G [3, Theorem 4.1], it is not surprising to see that in general quite different constructions have to be chosen in order to obtain graphs with a given number of vertices and edges having either a good permeability or a high value of $\varrho(A)$. If e.g. we have 7 vertices and 6 edges, the most permeable graph that can be constructed from this material is $K_{1,6}$, whereas $\varrho(A)$ becomes maximal for a graph consisting of one copy of K_4 plus three isolated vertices.

6. Applicability to other transportation processes

After having discussed this special transportation process one might ask, whether other kinds of transportation processes could be described by spectral means too. It seems to be a necessary condition, however, for a process to have a description in spectral terms that the propagation of the particles (or forces) takes place from one vertex to all neighbouring vertices vertices without leaving out vertices that e.g. "lie in the wrong direction".

Therefore it does not appear to be a promising attempt looking for a spectral description e.g. of the behaviour of passengers in nationwide airline or railway networks.

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